Experimental and theoretical approach to aggregation behavior of new di-*N*-oxide surfactants in an aquatic environment.

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Streszczenie

A homologous series of new dicephalic type surfactants (*N*,*N*-bis3,3′-(dimethylamino)propyl]alkylamide di-*N*-oxides) were synthesized and their aggregation phenomena were extensively studied. First, the pH-sensitivity of the investigated surfactants was tested in potentiometric titrations. Then, the adsorption isotherms were measured and interpreted using the Gibbs adsorption equation to determine physicochemical properties. The spin probe EPR technique was employed to monitor the micellization behavior of the surfactants, depending on temperature and surfactant concentration. Critical micelle concentrations (CMC) were determined through an analysis of the calculated spin probe rotational correlation times. A greater insight into the local microenvironment of the formed aggregates was gained by analyzing the properties of the immobilized spin probes. In addition, the CMC values were compared with the ones obtained from tensiometry measurements (taking into account the contributions of the various ionic and nonionic surfactant forms). The approximate size of the micellar aggregates was estimated by the dynamic light scattering (DLS) method. Good agreement between the experimental hydrodynamic radii and those predicted using density functional theory (DFT) guaranteed that the subsequently calculated aggregation numbers, representing the number of molecules in a micelle, were close to the real values. Moreover, the theoretical QSAR methods were used to determine the shape of the micelles via the prediction of the critical packing parameter (CPP).

Adres publiczny

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https://www.acs.org/content/acs/en.html